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13. ABSTRACT (Maximum 200 words)

The central focus of the program was on the application and development of modern analytical and computational methods to the solution of nonlinear problems in fluid dynamics and reactive gas dynamics. The research was carried out within the Division of Engineering Mathematics in the Department of Mechanical Engineering and Mechanics and principally involved Professors P A Blythe, E Varley and J D A Walker. In addition, the program involved various international collaborations. Professor Blythe completed work on reactive gas dynamics with Professor D Crighton FRS of Cambridge University in the United Kingdom. Professor Walker and his students carried out joint work with Professor F T Smith, of University College London on various problems in unsteady flow and turbulent boundary layers.

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FINAL REPORT

COMPUTATIONAL AND ANALYTICAL METHODS IN NONLINEAR FLUID DYNAMICS

AFOSR-89-0487

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September, 1993

1. Introduction

This is the final report on the URI project entitled "Computational and Analytical Methods in Nonlinear Fluid Dynamics" started in 1989 at Lehigh University in the Department of Mechanical Engineering and Mechanics. The present report summarizes work completed, as well as still in progress, at the end of the funding. The central focus of the program was on the application and development of modern analytical and computational methods to the solution of nonlinear problems in fluid dynamics and reactive gas dynamics. The research was carried out within the Division of Engineering Mathematics in the Department of Mechanical Engineering and Mechanics and principally involved Professors P. A. Blythe, E. Varley and J. D. A. Walker. In addition, the program involved various international collaborations. Professor Blythe completed work on reactive gas dynamics with Professor D. Crighton F.R.S. of Cambridge University in the United Kingdom. Professor Walker and his students carried out joint work with Professor F. T. Smith, F.R.S. of University College London on various problems in unsteady flow and turbulent boundary layers. This research will be briefly summarized subsequently.

A major portion of the work carried out under the contract was computational and concerned the incorporation of analytical local solutions into computational algorithms. In accordance with the theme of the URI program to enhance University infrastructure, two Silicon Graphics 4D25 workstations were purchased with contract funds. These computers were connected to the University network in a computational lab principally assigned to fluid mechanics research. They received extensive usage over the course of the contract and are still regularly used on a daily basis by graduate students and faculty.

During the contract period, four graduate students were funded (in full or in part) for studies toward their Ph.D. These students were supervised by Professor J. D. A. Walker and at present one Ph.D. has been awarded; the three other students will receive their Ph.D's in December, 1993. The students and their thesis topics are as follows:

(1) Ammar T. Degani, Ph.D. 1991, "The Three-Dimensional Turbulent Boundary Layer - Theory and Application".

(2) Kevin Cassel, Ph.D. (expected) 1993, "Interactive Boundary Layers".

(3) Jun He, Ph.D. (expected) 1993, "High-Speed Compressible Turbulent Boundary Layers".

(4) R. I. Puhak, Ph.D. (expected) 1993, "Flow Structure Upstream of Three-Dimensional Obstacles".

Mr. Cassel and Mr. Puhak are American citizens while Dr. Degani is a residential alien. Dr. Degani recently won a Nason Postdoctoral Fellowship in Parallel Processing at Syracuse University, while Mr. Cassel was successful in a competition for a Postdoctoral Fellowship at NIST in Combustion Studies.

In the following sections, research carried out under the grant is briefly summarized; more detail is available in the publications summarized at the end of this report.

2. Description of Research

A. Professor J. D. A. Walker

A.1 Analytical and Computational Studies of Unsteady Separation

Associated Graduate Student: Kevin Cassel

Status: Ph.D., draft of thesis complete, expected graduation December 1993.

Unsteady separation of boundary layers occurs in a variety of physical situations such as dynamic stall in rapidly pitching airfoils, vortex shedding in turbines and eruption of the wall layer in transitioning and turbulent boundary layers. Until relatively recently, the nature and causes of this phenomena at high Reynolds numbers have not been well understood. The Ph.D. thesis of Van Dommelen (1981) and subsequent theoretical work by Elliott et al. (1983) revealed that in two-dimensional flows, a generic response develops within a thin boundary-layer flow that is exposed to a persistent adverse pressure gradient. The influence of viscosity first leads to the evolution of recirculating flow within the boundary layer and if the external adverse pressure gradient is maintained, a sharply focussed eruption of the surface layer develops abruptly at a subsequent time. The calculation of such flows, using conventional numerical methods based on the Eulerian description of the flow field, is not possible owing to the rapid development of a "spike-like" eruption of the surface flow. Van Dommelen (1981) was able to calculate the evolution of the boundary layer

on an impulsively-moved circular cylinder through the use of Lagrangian methods, wherein the trajectories of a large number of individual fluid particles were calculated. In this manner, it proved possible to track the phenomenon up to the formation of a sharp spike in displacement thickness. The theoretical account of Elliott et al. (1983) suggests that the formation of the "spikes" is a generic state passed through by most erupting boundary layers at high Reynolds numbers. Recently, this suggestion has been supported by numerical solutions of the boundary layer induced by a vortex above a plane wall, carried out by Peridier et al. (1991a, 1991b). In the limit of large Reynolds numbers, the vortex-induced separating boundary layer evolves toward a singularity structure which is essentially similar to that described by Elliott et al. (1983). As the singularity structure develops, the external flow field must be allowed to change and reflect the fact that boundary-layer vorticity is now shooting rapidly toward the outer region.

Because unsteady separation at high Reynolds numbers is pervasive in aeronautical applications, it is important to develop an understanding of the steps that occur in the process as a separating boundary layer leaves the surface. Until recently, it was believed by many authors that the problem could be handled using conventional interacting boundary layer concepts. The present research has definitively shown that this is not the case and that more sophisticated algorithms will be required for this important problem. In 1983, Elliott et al. formulated a boundary value problem describing what we refer to as the first interactive stage; this occurs just prior to the evolution of a singularity in the non-interactive problem and is the first stage wherein the external flow is influenced by the rapidly thickening viscous region near the surface. The unsteady boundary-value associated with this stage is extremely complex from a numerical standpoint owing to difficulties associated with the boundary conditions.

The first numerical solutions for the first interactive stage were obtained in the present program. By recasting the problem in a Lagrangian formulation, it proved possible to formulate a numerical algorithm that would accurately calculate the flow development in the first interactive stage. Initially, it was expected that the solution would evolve toward another singularity but repeated calculations revealed the evolution of a high frequency instability. As the meshes were refined, this instability was found to occur at progressively earlier stages. Repeated checks on the numerical work and analysis of the instability were carried out. This work has shown that the instability is not numerical but appears to be a new type of interactive instability. It is primarily inviscid in nature but does not involve an inflectional velocity profile. A

paper on this discovery has been submitted to the *Journal of Fluid Mechanics* (Cassel, Smith & Walker, 1993).

A.2 Embedded Function Methods for Three-Dimensional Turbulent Boundary Layers
Associated Graduate Student: A. T. Degani
Status: Ph.D. awarded in October, 1991

In most conventional methods for the calculation of three-dimensional turbulent boundary layers, the majority of computational time and resources is invested in resolving the severe gradients in the velocity and temperature gradients that occur in the near-wall region. In the present research asymptotic analysis was used to develop local analytical solutions that could be embedded in a general computational scheme for the turbulent boundary layer. In the papers by Degani et al. (1992, 1993), the method of matched expansions was used to determine the general asymptotic structure of an attached three-dimensional turbulent boundary layer. This work established for the first time that the inner wall layer exhibits an essentially universal self-similar behavior and the matching conditions for the velocity profiles near the edge of the wall layer were determined. A set of analytical profiles that can be used in the turbulent wall layer in a computational algorithm were developed. The concept was demonstrated in a three-dimensional boundary-layer prediction code (Degani & Walker, 1993) where the analytic embedded functions were used to "step over" the turbulent wall layer in a calculation. In this manner, it is only necessary to carry out a computation in the outer part of the boundary layer and, skin friction and heat transfer coefficients are determined through matching to the analytic embedded functions. Through use of asymptotic theory and the embedded function methodology, it has proved possible to construct a much more efficient algorithm for turbulence prediction near walls in which the total number of mesh points used may be reduced by about 50% (as compared to a conventional method) with no degradation in accuracy.

A.3 Modeling of Supersonic and Hypersonic Turbulent Boundary Layers
Associated Graduate Student: Jun He
Status: Thesis draft complete, Ph.D. expected December, 1993.

Supersonic and hypersonic turbulent boundary layers occur in a variety of important aerodynamic applications. Unfortunately, most turbulence models for high-speed compressible flow are based upon ad hoc extensions of turbulence models that have been correlated to represent subsonic data. As the Mach number of the

mainstream flow increases, the structure of the turbulent boundary changes and a new physical effect becomes important, namely dissipation of kinetic energy near the surface into heat energy. Unfortunately, there are few reliable measurements of the temperature distribution in the supersonic/hypersonic flow regime or even of the turbulence quantities themselves. Existing turbulence models currently in use can easily be shown to be incompatible with experimental data as well as inconsistent in the asymptotic limit of high Reynolds number flows.

The objective of this research was to determine the asymptotic structure of a high-speed compressible turbulent flow in the limit of large Reynolds numbers and further to develop simple turbulence models which can predict skin friction and heat transfer coefficients. The study of He et al. (1992) reports the development of a self-consistent mathematical asymptotic structure for high-speed compressible turbulent boundary layers. In this paper the adiabatic wall was considered and an analytical expression was derived for the recovery factor. New and simple turbulence models were obtained, and a direct comparison with experimental data showed excellent agreement for both the velocity and total enthalpy data. Subsequent work has incorporated the influence of heat transfer with the new models and also to extend the theory into the hypersonic regimes. The theory described in He et al. (1992) is valid for mainstream Mach numbers up to about 6.

A.4 Unsteady Three-Dimensional Separation

Associated Graduate Student: Robert Puhak

Status: Ph.D. expected in December, 1993.

Recent advances in the theory of unsteady separation (Van Dommelen & Cowley, 1990; Cowley et al. 1991) have suggested that when a three-dimensional boundary layer undergoes a process of unsteady separation from a surface, a generic structure develops in a high Reynolds number flow. It is suggested that the eruption takes the form of a sharply focussed tongue of fluid that moves rapidly away from the surface. In three-dimensional flows, boundary-layer separation is believed to initiate somewhere along the surface of zero vorticity (where both the transverse and streamwise vorticity components vanish simultaneously). However, numerical work on three-dimensional separated flows is rather limited. The objective of this research is to calculate the evolution of some fundamental problems involving three-dimensional unsteady separation of a surface boundary-layer. The goal is to track the evolution of the different types of recirculations that can develop and from this determine how the

layer evolves toward an eruption.

A model problem under consideration consists of a circular cylinder mounted on a flat surface and a high speed flow moving steadily from left to right. This geometry represents a generic type of configuration occurring in a large number of situations (wing/air frame junctures, turbine blade base flows, for example), and it is important to understand the dynamics of such regions. At present numerical solutions for the developing flow on the upstream and downstream symmetry plane have been obtained. The upstream symmetry plane is of particular interest since here the adverse pressure gradient due to the cylinder gives rise to unsteady separation in the end-wall boundary-layer. The present computations for the developing boundary layer on the end wall are among the first to be carried out in three dimensions in Lagrangian coordinates. Calculated results show the evolution of a complex separation singularity (Degani, Puhak & Walker, 1993).

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B. Professor E. Varley

B.1 Applications of Some Exact Solutions to the Navier-Stokes Equations

Two families of exact solutions to the Navier-Stokes equations (NSE) have been used to analyze some technically important flows. The first family, designated F1 flows, is characterized by the fact that the component of fluid velocity in the direction normal to some plane is a function only of time, t, and the distance, y, from that plane. The plate can rotate and translate with time varying velocities. In addition to being exact solutions to the NSE, the F1 solutions are exact solutions to the boundary-layer equations (BLE): the terms that are usually omitted to obtain the BLE from the NSE are identically zero. Well-known examples of parallel F1 flows are Couette (1890), Rayleigh (1911) and Ekman (1905) flows. Examples of non-parallel flows are the various von Karman (1921) swirling flows, and the Blasius-Hiemenz (1908, 1911) flow at a forward stagnation point. In these examples, either the fluid is contained between two parallel plane surfaces, or occupies a semi-infinite region bounded by a single plane surface. For Couette and Rayleigh flows, the bounding surfaces translate in directions parallel to their planes, but do not rotate; for Ekman flows the bounding surfaces rotate about the same fixed axis with the same constant total angular velocity and translate in directions parallel to their planes. von Karman flows are generated when two parallel plane surfaces rotate with different angular speeds about a common, fixed axis that is normal to their planes. The Blasius-Hiemenz flow approximates that produced near a line of symmetry when a fluid is squeezed between two parallel plates moving with different speeds normal to their planes.

All the viscometric-type flows listed above are produced when the motions of the bounding plane surfaces have at most two degrees of freedom. The F1 solutions to the NSE obtained in the course of this research may be used to describe flows that are produced when the bounding surfaces move in *any* manner that is compatible with the remaining plane, rigid and parallel: they can translate in directions parallel and normal to their planes and rotate about different axes. The mathematical problem reduces to that of solving a set of PDE in the two independent variables (t,y). This can be split into two sets; the first set, which is usually nonlinear, describes the primary component of the flow and is identical to that governing one of the flows listed above: it uncouples from the second set which, essentially, is linear with coefficients that are determined by the primary component of the flow. Two sub-classes of F1 flows are of special interest because they involve relatively simple mathematics. The simpler one is characterized

by the fact that the primary component is such that the coefficients in the second set of linear PDE are functions only of t. These equations can be transformed into two, uncoupled, constant coefficient diffusion equations. For the second sub-class of F1 flows, the primary component of the flow is steady and is governed by a set of nonlinear ODE; the second set of linear equations have coefficients that are functions only of y.

The second family, the F2 flows, are generalized plane flows in the sense that, if (x_1, x_2, y) denote the Cartesian co-ordinates of a point in the fluid at which the velocity components are (u_1, u_2, v), the u_i are independent of y. One example is Poiseuille (1984) pipe flow, for which the $u_i \equiv 0$ and $v = v(x_1, x_2)$; another is the Burer (1941) vortex flow, for which $v = v_1 y$ and the flow is radially symmetric about the y-axis. As another example, we have analyzed unsteady, radially symmetric, F2 flows for which $v = v_1(t,r)y + v_o(t,r)$. These are produced near the outer surface of a circular cylinder whose velocity varies in time: the surface may rotate with a time varying angular velocity, translate with a time varying velocity in the direction parallel to the axis of the cylinder, and expand or contract with a time varying velocity in the radial direction. Away from the cylinder the flow asymptotes to that in an unsteady Burger vortex.

The main result of this research has been to show how the F1 solutions of the NSE may be used to analyze some features of the strong local interaction between a thin shear layer, in which the flow is initially parallel, and a disturbance in the outer mainstream. An excellent example of such a problem occurs in the study of the strong *local* atmospheric disturbance that is produced in a layer of air, where the flow is strongly sheared, by the passage of a tornado. Here, the lower boundary of the layer, representing the earth, is fixed and the upper boundary, representing the cloud base, is rotating and translating. Mainly, we have concentrated on the flow in regions away from material boundaries where it is the fact that the fluid is strongly sheared that controls the interaction with the mainstream flow and not the presence of rigid boundaries. In this sense the layer is a free shear layer, and the governing equations can be transformed into constant coefficient diffusion equations.

The solutions to the NSE equations describing F1 flows may be used only to describe the local behavior of global flow solutions that must be determined either numerically or by using approximate equations. These approximate equations are obtained by noting that these global flows are often well-described by solutions of the BLE in which the pressure $p(t, x_1, x_2)$ can be estimated a priori. Moreover, away from rigid boundaries, even though the flow is strongly sheared, the viscous terms in the BLE

are unimportant and can be omitted. We have described a procedure that can be used to integrate the resulting hydraulic flow equations (HFE). This involves reformulating the equations in terms of Lagrangian variables, thus reducing the problem of solving a system of nonlinear PDE to that of solving a system of nonlinear ODE. In the special case of F1 flows, the pressure gradient terms, $\partial p/\partial x_i$, are linear forms in the x_i with coefficients that depend on t. The resulting ODE are linear, and a general representation for the flow variables, which are also exact solutions for the Euler equations (EE), can be found. These solutions are used to show that unless $p(t, x_1, x_2)$ is estimated with care, the F1 solutions to both the EE and the NSE develop singularities in a finite time.

As an example of our general analysis we have described the flow that is produced at the edge of a shear layer during the passage of a Rankine vortex in the mainstream. Far from the layer the axis of the vortex is perpendicular to the layer and moves with a time varying velocity; the strength of the vortex also varies with time. This flow models that occurring in the center of a tornado which, far above the earth, is convected with the ambient wind-speed. The resulting flow is unsteady and fully three dimensional.

The F1 and F2 solutions of the NSE are exact solutions to flow problems that are highly idealized in that they involve boundaries of infinite extent. However, like the classical Rayleigh and von Karman solutions, sometimes they can be used to provide useful information about local condition in more complicated and realistic global flows. For example, F1 flows can be used to approximate a real flow in the vicinity of an axis of rotation or a line of symmetry, while F2 flows can be used in the vicinity of some plane. The F1 and F2 solutions are *similarity* solutions of the NSE and, like other similarity solutions, must be interpreted with care: they can be used only when it can be argued that the local flow is well approximated by a viscometric flow.

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C. Professor P. A. Blythe

C. Wave Induced Ignition

C.1 Introduction

Exothermic reactions, with Arrhenius kinetics, depend exponentially on the activation energy. In many cases this characteristic energy is relatively large and rapid thermal heating occurs. Over the induction period prior to ignition the evolution of small gas dynamic disturbances is governed by the Clarke equation (Clarke 1981, see §C.2). Analytical progress with this equation is difficult. Numerical solutions for semi-infinite domains in which the reaction is switched on by the passage of a shock of finite strength have been obtained by Clarke & Cant (1985) and by Jackson & Kapila (1985). More recently, Blythe & Crighton (1989)[1] developed an asymptotic approach based on the Newtonian limit $\gamma \to 1$ where γ is the frozen specific heat ratio. Excellent agreement with the numerical calculations is found.

More complex problems arise when the motion is generated in a finite domain by an initial (weak) non-uniform temperature distribution. The ignition stage of these disturbances is a precursor to the development of a local hot spot into a fully fledged thermal exposition, and is again governed by Clarke's equation. Jackson, Kapila & Stewart (1989) have investigated this class of problems by using co-ordinate expansions combined with computational techniques. As in the shock generated problem, analytical progress is difficult.

The research carried out under this part of the grant was concerned with extending the Newtonian approach to examine:

(1) non-linear hot-spot structure and the reaction wave speed (§C.3);

(2) influence of upstream disturbances on shock induced ignition (§C.4);

(3) spatio-temporal evolution of thermal irregularities in bounded domains (§C.5).

These problems have direct bearing on fundamental problems related to the birth of detonation waves and the onset of thermal explosions in confined vessels. Combustion-driven disturbances that propagate into non-uniform regions, possibly far from thermodynamic equilibrium, also arise in flow fields that are characteristic of proposed hypersonic transports.

[1] Hereafter referred to as BC.

C.2 The Clarke Equation

Small disturbance theory at high activation energies ϵ^{-1} is governed by a distinguished limit in which the disturbance amplitude is $O(\epsilon)$. Here ϵ^{-1} is a dimensionless measure relative to a background state characterized by a (dimensionless) temperature $T = 1$. Over the induction time scale local solutions can be expanded in the form

$$T = T_o + \epsilon T_o^2 T_1(x,t) + \ldots, \tag{C.2.1}$$

where T_o is either unity or the initial temperature behind any reaction-inducing shock. After suitably scaling the spatial co-ordinate x and the time t, the temperature perturbation T_1 can be shown to satisfy Clarke's equation

$$\left(\frac{\partial^2}{\partial t^2} - \gamma\frac{\partial^2}{\partial x^2}\right)\frac{\partial T_1}{\partial t} - \left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)e^{T_1} = 0. \tag{C.2.2}$$

In (C.2.2) the high frequency operator is associated with the frozen wave speed $\gamma^{1/2}$ and the low frequency operator with the isothermal (Newtonian) speed ($\equiv 1$ in current variables).

Although general analytical solutions of (C.2.2) do not appear to be possible, progress has been made in the Newtonian limit $\gamma \to 1$. To leading order the wave equation (C.2.2) degenerates into

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)\left(\frac{\partial T_1}{\partial t} - e^{T_1}\right) = 0, \tag{C.2.3}$$

which can be integrated. However, as shown in BC for shock-induced ignition, this result is not uniformly valid near the ignition point (hot spot) where local adjustments take place in a region that is exponentially thin with respect to $\gamma - 1$. Discussion of the structure near the hot spot is reported in §C.3. Note that this analysis follows BC and uses the ordered limit

$$1 \gg \gamma - 1 \gg \epsilon, \tag{C.2.4}$$

whereas the derivation of (C.2.2) is dependent only on the assumption that $\epsilon \ll 1$.

Modification of the Newtonian analysis given in BC is also required when (C.2.4) is replaced by

$$\gamma - 1 = O(\epsilon) = o(1). \tag{C.2.5}$$

For this limit, the Clarke equation is still valid, but the ignition time upstream of the shock is now comparable with that downstream of the shock. Consequently, thermal excitation ahead of the shock must be included in the analysis. Basic results, including corrections to the ignition time, are outlined in §C.4.

As noted in the Introduction (§C.1), equation (C.2.2) also governs the evolution of initial spatial thermal irregularities in bounded domains. The amplification of local hot spots in such flows has been examined by Jackson, Kapila & Stewart (1989) when $\gamma - 1 = O(1)$. An analytical approach, based on the Newtonian limit (C.2.4), is described in §C.5.

C.3 Hot Spot Structure and Wave Speed

For shock induced ignition, the disturbance is initiated by a piston moving at finite speed. Using expansions of the form (C.2.1), the small disturbance equations can be written in characteristic form as

$$\partial_{\pm}(p_1 \pm v_1) = e^{T_1}, \tag{C.3.1}$$

with

$$\partial_{\pm} \equiv -\frac{\partial}{\partial \tau} \pm \frac{\partial}{\partial \xi}. \tag{C.3.2}$$

Here p_1 is the pressure perturbation, v_1 is the velocity perturbation (relative to the piston speed), ξ is the distance from the piston face, and the time to ignition

$$\tau = t_i - t, \tag{C.3.3}$$

where t_i is the ignition time on the piston face and must be determined as part of the solution. The exponential term on the right-hand side of (C.3.1) represents the strong influence of exothermic heating. Similarly, along the particle paths

$$\frac{\partial T_1}{\partial \tau} - \delta \frac{\partial p_1}{\partial \tau} - = (1 - \delta)\, e^{T_1}. \tag{C.3.4}$$

with

$$\delta = (\gamma - 1)/\gamma. \tag{C.3.5}$$

These results are based on a one-step first order reaction with Arrhenius kinetics, and the corresponding reduced rate law for the perturbation mass fraction y_1 is

$$\beta\frac{\partial y_1}{\partial \tau} = e^{T_1}, \tag{C.3.6}$$

where β is a dimensionless formation energy.

Newtonian expansions of the small disturbance equations correspond to the subsequent limit $\delta \to 0$ and, prior to ignition, have the form

$$T_1(\xi, \tau; \delta) = T_{10}(\xi,\tau) + \delta T_{11}(\xi,\tau) + \ldots \tag{C.3.7}$$

etc. Substitution into (C.3.1) – (C.3.6) shows that the solution for the leading order terms can be written

$$\left.\begin{aligned} T_{10} &= -\beta y_{10} = -\ell n(\tau + v^{-1}\xi) \\ p_{10} &= \frac{V^2}{1-V^2}\,\ell n(\tau + V^{-1}\xi) + f(\tau+\xi) + g(\tau+\xi) \\ v_{10} &= \frac{V}{1-V^2}\,\ell n(\tau + V^{-1}\xi) + f(\tau+\xi) - g(\tau-\xi) \end{aligned}\right\} \tag{C.3.8}$$

where

$$V = \left[\frac{(\gamma-1)M_o^2+2}{2\gamma M_o^2-(\gamma-1)}\right]^{1/2}\left(\simeq \frac{1}{M_o}\right) \tag{C.3.9}$$

and M_o is the initiating shock Mach number. Determination of the functions $f(\tau)$ and $g(\tau)$ requires implementating of suitable shock relations along the shock path

$$\xi = V(t_i - \tau). \tag{C.3.10}$$

Solutions of the resulting functional equations can be expressed in the form

$$\left.\begin{aligned} f(\tau) &= -\frac{(1-\lambda^2)}{4\lambda}\sum_{n=1}^{\infty}(-N)^n\,\ell n[1-\lambda^n(1-\tau)] \qquad (\tau > 0) \\ g(\tau) &= -\frac{(1-\lambda^2)}{4\lambda}\sum_{n=1}^{\infty}(-N)^n\,\ell n[1-\lambda^n(1-\tau)] \qquad (\tau > -V) \end{aligned}\right\} \tag{C.3.11}$$

with

$$\lambda = \frac{1-V}{1+V}, \quad N = \frac{1-R}{1+R}, \quad R = \frac{2M_o^2}{M_o^2+1} V. \tag{C.3.12}$$

Note that $1 > \lambda > 0$, $1 > N > 0$.

Further details can be found in BC, together with determination of higher order corrections. In particular, it is shown that the ignition time

$$t_i = 1 + a\delta + \ldots, \tag{C.3.13}$$

where

$$a = \frac{(1+\lambda)}{2\lambda} - 2\int_o^1 f(\tau)d\tau. \tag{C.3.14}$$

From (C.3.8) it can be seen that the solution has a logarithmic singularity at $\tau = 0$ on the piston face $\xi = 0$. In fact (C.3.8) suggests that the singularity propagates along

$$\tau = -V^{-1}\xi,$$

but this concerns events for $\tau < 0$ $(t > t_i)$ where the above small disturbance theory is not valid.

The basic Newtonian expansion (C.3.7) fails near the hot spot $\xi = \tau = 0$, and it is convenient to introduce a centered co-ordinate

$$\chi = \xi/\tau. \tag{C.3.15}$$

From (C.3.8), the limiting behavior of the outer temperature becomes

$$T_1 \sim -\ell n\, \tau - \ell n\, (1 + V^{-1}\chi) + O(\delta). \tag{C.3.16}$$

Newtonian small disturbances theory also predicts that the remaining thermodynamic variables, including the density, have logarithmic singularities on the piston face at $\tau = 0$. Near $\xi = \tau = 0$ it is necessary to introduce $(\tau > 0)$ a nonlinear stretched time through

$$\sigma = -\ell n\ \bar{c}\ (\tau = \exp(-\sigma/\delta)) \tag{C.3.17}$$

and to seek local expansions

$$\left.\begin{aligned} T_1 &= \frac{\sigma}{\delta} + \theta(\chi, \sigma; \delta), \\ p_1 &= \frac{\psi(\sigma)}{\delta} + P(\chi, \sigma; \delta), \\ v_1 &= U(\chi, \sigma; \delta), \end{aligned}\right\} \tag{C.3.18}$$

etc.

It is not difficult to show that the leading approximations to θ is given by

$$\theta_o = -\ell n[1 + C(\sigma)x]. \tag{C.3.19}$$

Here $C(\sigma)$ is defined implicitly by

$$Ce^C = V^{-1} \exp\,[V^{-1} - \sigma], \tag{C.3.20}$$

and the derivation of (C.3.20) requires extending the analysis to second order terms (see BC). Related results for the remaining dependent variables can also be obtained. In particular, the leading order velocity

$$U_o = \frac{C}{1 - C^2}\ \ell n\left[\frac{1+\chi}{1+C\chi}\right], \tag{C.3.21}$$

which, as required, vanishes on $\chi = 0$. Further, the logarithmic singularity in the outer density is replaced by a bounded limit as $\sigma \to \infty (\tau \to 0)$, which is consistent with the numerical calculations of Jackson & Kapila and Clarke & Cant.

The representation (C.3.18) is not valid across $\tau = 0$, i.e. in $\tau < 0$ (see (C.3.17)). To extend the solution into $\tau < 0$ it is necessary to introduce

$$\xi = e^{-s/\delta}, \qquad r = \tau/\xi = \frac{1}{\chi}. \tag{C.3.22}$$

so that in $\tau > 0$ $(r > 0)$

$$\sigma = s - \delta \ \ell n \ r. \tag{C.3.23}$$

Either directly from the governing equation, or by re-expressing (C.3.19) – (C.3.21) etc. in terms of s and r, it can be shown that

$$T_1 = \frac{s}{\delta} - \ell n \ [r + C(s)] + \frac{\delta}{r + C(s)} \left[\frac{C(s)}{1 + C(s)} \left\{ r - \ell n \ (1 + r) \right\} + \Gamma_1(s) \right] + \ \ldots \tag{C.3.24}$$

with corresponding results for the other dependent variables. The expression (C.3.24) is valid in $r < 0 (\tau < 0)$. In general, this form of the solution is not uniformly valid as $r \to \infty$ (i.e. on the piston face with $\tau < 0$), unlike the formulation (C.3.18), which is valid on $\xi = 0$ for $\tau < 0$. The representations in terms of (s, r) and (σ, χ) do, however, overlap for $r = 0(1)$.

From (C.3.24), it appears that the ignition path is defined by the logarithmic singularity on

$$r = r_i = - C(s), \tag{C.3.25}$$

although the term $0(\delta)$ has a stronger algebraic singularity along this path. Results obtained by Friedman & Herrero (1989) imply that the Clarke equation can at most have a logarithmic singularity at ignition. This suggests using a PLK approach to define ignition through

$$r_i = - C(\bar{s}) \tag{C.3.26}$$

with

$$s = \bar{s} \ + \delta s_1(\bar{s}) + \ \ldots \ . \tag{C.3.27}$$

$s_1(\bar{s})$ is now chosen to eliminate the algebraic singularity which requires

$$s_1 = - C - \ell n(1 - C) + \frac{(1 + C)\Gamma_1(C)}{C} . \tag{C.3.28}$$

Using this result, and (C.3.26), it can be established that the reaction wave speed

$$\frac{d\xi_i}{dt} = \frac{1}{C} \left[1 - \delta \left\{ \frac{\Gamma_1(C)}{C} - \frac{\ell n(1 - C)}{1 + C} \right\} + \ \ldots \right], \tag{C.3.29}$$

where now $C = C(s)$. Note that the wave speed becomes unbounded on the piston face ($\xi = 0$ or $s = \infty$, implying $C = 0$); this is consistent with numerical prediction for the Clarke equation.

Internal to the present region, which is exponentially thin with respect to δ, the complete structure for the full equations includes a fuel consumption zone that is exponentially thin in ϵ. Corresponding extensions for the full wave structure are planned.

The result (C.3.28) also fails near $C = 1$ where the wave speed is equal to the speed of the outgoing characteristic leaving the hot spot. Note also that the temperature solution (C.3.24) has a logarithmic singularity on this characteristic ($r = -1$), but the present inner solution is valid only in $r > -C(s)$ with $C < 1$.

Resolution of these difficulties requires an analysis of the full equations, including fuel consumption, and is an essential step in providing a complete description of the ultimate evolution of any detonation wave. Future research will examine this structure.

C.4 Upstream Heat Release

If the ordered limit (C.2.4) is replaced by

$$1 \gg \gamma - 1 = 0(\epsilon), \tag{C.4.1}$$

then modifications must be made to the analysis described in §C.3. Using the expansion (C.2.1), with

$$y = 1 + \epsilon\, T_o^2\, y_1(\xi, \tau) + \ldots, \tag{C.4.2}$$

the full rate law

$$\partial_\tau y = -\epsilon\, \beta^{-1}\, y \exp\left[\frac{1}{\epsilon}\left(\frac{1}{T_o} - \frac{1}{T}\right)\right] \tag{C.4.3}$$

reduces to (C.3.6) downstream of the shock. In general, exothermic heating will also occur upstream of the shock. Suitable local expansions are

$$\left.\begin{aligned} T_1 &= 1 + \epsilon T_{1\infty}(t) + \ldots \\ y_1 &= 1 + \epsilon y_{1\infty}(t) + \ldots \end{aligned}\right\} \qquad \text{(C.4.4)}$$

with $p_{1\infty} = T_{1\infty}$ and $\rho_{1\infty} = u_{1\infty} = 0$. It is readily established that

$$\frac{dT_{1\infty}}{dt} = \frac{1}{t_\infty} e^{T_{1\infty}}, \qquad \text{(C.4.5)}$$

where

$$t_\infty = \exp\left[\frac{1}{\epsilon}\left(\frac{T_o - 1}{T_o}\right)\right]. \qquad \text{(C.4.6)}$$

When $\gamma - 1 = O(\epsilon)$, the standard shock relations imply that $T_o - 1 = O(\epsilon)$, so that $t_\infty = O(1)$, i.e. ignition times upstream of the shock are now comparable with those downstream of the shock.

For convenience, it is supposed that the shock is initiated at $t = t_o$ and propagates into the region $x > 0$. The upstream reaction is assumed to start at $t = 0$ with an initial state

$$T = p = \rho = y = 1, \quad u = 0.$$

Consequently, from(C.4.5)

$$T_{1\infty} = -\ell n\left(1 - \frac{t}{t_\infty}\right). \qquad \text{(C.4.7)}$$

Obviously, for the current analysis to be appropriate, $t_\infty > t_o$.

The solution downstream of the shock is still governed by the Clarke equation, but conditions on the shock path

$$\xi = V(\bar{t}_i - \tau), \quad (\bar{t}_i = t_i - t_o) \qquad \text{(C.4.8)}$$

must be modified. In particular, the relationship between the temperature and velocity perturbations is

$$T_{s1} = \delta Q v_{s1} + Q_\infty T_{1\infty}, \tag{C.4.9}$$

where

$$Q = \frac{2(\gamma M_o^4 + 1)V}{(M_o^2 + 1)((\gamma - 1)M_o^2 + 2))}, \tag{C.4.10}$$

$$Q_\infty = 1 - \delta q_\infty, \tag{C.4.11}$$

and

$$q_\infty = \frac{2\gamma}{(\gamma+1)^2} \frac{(M_o^2 - 1)(\gamma(\gamma+1)^2 M_o^6 + \gamma(\gamma-1)M_o^4 + \gamma(\gamma+5)M_o^2 + 2)}{M_o^2\,[(\gamma-1)M_o^2 + 2]}. \tag{C.4.12}$$

Similarly,

$$P_{s1} = R v_{s1} + R_\infty T_{1\infty}, \tag{C.4.13}$$

with

$$R_\infty = \frac{(3\gamma+1)M_o^2 - (\gamma-1)}{(\gamma+1)\rho_o T_o^2 (M_o^2+1))}. \tag{C.4.14}$$

Here the coefficients denoted by a subscript ∞ are associated with the upstream behavior.

From these results, the leading order solution for the temperature perturbation is found to be

$$T_1 = -\ell n\,[\tau + (1 - t_o^{-1})V^{-1}\xi]. \tag{C.4.15}$$

In addition, relative to shock initiation, the ignition time is

$$t_i - t_o = 1 - \frac{t_o}{t_\infty}. \tag{C.4.16}$$

Corresponding results for the velocity and pressure perturbation have been determined

and can be written down in a form similar to (C.3.8) and (C.3.11). Similarly, extensions of the analysis to describe the hot spot structure have been carried out using the approach described in §C.3. Calculations of higher order corrections to the temperature distribution and the ignition time are partially complete.

C.5 Ignition from a Spatially Distributed Source

(a) Basic Theory

For a spatially uniform initial state, ignition should ideally occur in a spatially homogeneous manner. Weak irregularities in the background thermal field, however, can lead to local hot spots that become energetic centers associated with the development of a thermal explosion. Problems of this type have been considered for bounded domains ($0 \le x \le \ell$) by Jackson, Kapila & Stewart (1989)[2]. Over the induction phase, prior to ignition, it can be shown that the disturbance is still governed by Clarke's equation.

In this section the variables adopted will follow those introduced by JKS. Relative to (C.2.2), the coordinates (x,t) are now replaced by ($\gamma^{3/2}x$, γt) and the Clarke equation becomes

$$\left(\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}\right)\left(\frac{\partial T_1}{\partial t}\right)-\left(\gamma\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}\right)e^{T_1}=0. \tag{C.5.1}$$

Similarly, the results (C.3.1) and (C.3.4) can be re-written as

$$\left(\frac{\partial}{\partial t}\pm\frac{\partial}{\partial x}\right)\left(p_1\pm\gamma u_1\right)=\gamma e^{T_1} \tag{C.5.2}$$

$$\frac{\partial T_1}{\partial t}-\delta\frac{\partial p_1}{\partial t}=e^{T_1}, \tag{C.5.3}$$

with, as before, $\delta=(\gamma-1)/\gamma$. It is assumed that there is an initially thermal non-uniformity of size ϵ so that

$$\left.\begin{aligned} &T_1(x,0)=\theta(x/\ell)\\ \text{with}\quad &\\ &p_1(x,0)=u_1(x,0)=0. \end{aligned}\right\} \tag{C.5.4}$$

[2]Hereafter referred to as JKS.

In addition, the velocity must satisfy

$$u_1(0,t) = u_1(\ell,t) = 0. \tag{C.5.5}$$

For convenience, the domain $0 \le x \le \ell$ is mapped onto the unit interval by introducing

$$(x,t) \Rightarrow \ell(x,t), \tag{C.5.6}$$

together with

$$\left.\begin{aligned} &T_1 \Rightarrow T_1 - \ell n\ \ell, \quad \rho_1 \Rightarrow \rho_1 + \ell n\ \ell \\ &p_1 \Rightarrow p_1, \quad u_1 \Rightarrow u_1. \end{aligned}\right\} \tag{C.5.7}$$

Under this mapping, the basic equations are invariant. Boundary and initial data are also unchanged save that

$$T_1(x,0) = \theta_1(x) + \ell n\ \ell = \theta(x{:}\ell). \tag{C.5.8}$$

Newtonian expansions of the form

$$T_1 = T_{1o}(x,t) + \delta T_{11}(x,t) + \ \ldots \tag{C.5.9}$$

etc., are used to generate the small amplitude pre-ignition solution. As in §3, it is assumed that $1 \gg \delta \gg \epsilon$. The basic solutions for the temperature is easily shown to be

$$T_{1o} = -\ell n \left[t_e(x) - t\right], \tag{C.5.10}$$

where the apparent ignition locus

$$t_e(x) = \exp\{-\theta(x;\ell)\}. \tag{C.5.11}$$

Further analysis then gives

$$\left.\begin{aligned} 4p_{1o} &= f(\alpha) + f(\beta) + I_+(x,\alpha) - I_-(x,\beta) \\ 4u_{1o} &= f(\alpha) - f(\beta) + I_+(x,\alpha) + I_-(x,\beta) \end{aligned}\right\}, \tag{C.5.12}$$

where

$$I_\pm(x,r) = 2\int_o^x \frac{ds}{t_\ell(s) - (r \pm s)} \tag{C.5.13}$$

and

$$\alpha = t - x, \quad \beta = t + x. \tag{C.5.14}$$

The function f(t) can be found by application of the initial and boundary conditions. It follows that for $2n > t > 2n-1$,

$$f(t) = \sum_{m=1}^{n} J\Big(t - (2m-1)\Big) - I_+(2n-t,\, t-2n), \tag{C.5.15}$$

and for $2n+1 > t > 2n$,

$$f(t) = \sum_{m=1}^{n} J\Big(t - (2m-1)\Big) + I_-(t-2n,\, t-2n), \tag{C.5.16}$$

where

$$J(t) = 4\int_o^1 \frac{t_e(s) - t}{(t_e(s) - t)^2 - (1-s)^2}\, ds. \tag{C.5.17}$$

Note that for $-1 < t < 0$

$$f(t) = -I_+(-t,t). \tag{C.5.18}$$

This definition of f(t) can be used to provide a complete representation for the leading order solution.

As in the shock driven case, it is possible to obtain a higher order correction for the temperature distribution. This result also yields an important correction to the ignition time (see §C.5b). From (C.5.3), and the expansion (C.5.9),

$$\frac{\partial T_{11}}{\partial t} - \frac{\partial p_{1o}}{\partial t} = e^{T_{1o}}\, T_{11}.$$

Using (C.5.10), and $T_1(x,0) = p_{1o}(x,0) = 0$, leads to

$$T_{11}(x,t) = p_{1o}(x,t) + \frac{1}{t_e(x) - t} \int_o^t p_{1o}(x,s)ds. \qquad \text{(C.5.19)}$$

The solution defined by (C.5.10) – (C.5.19) fails near the hot spot on $x = 0$. Local solutions of the type discussed in §3 for the shock generated case can again be obtained in zones that are exponentially close to the hot spot. Details are given in Crighton & Blythe (1993). As in §3, the analysis described above holds only for $t < t_i$, where t_i is the minimum ignition time on the left end wall. Evolution of the reaction wave away from the hot spot is not described by the Clarke equation, and (C.5.11) does not provide an overall description of the ignition path. Results for the minimum ignition time on $x = 0$ are presented below in §C.5(b).

(b) Ignition times

Initial thermal disturbances considered by JKS were of two types:

Type B is characterized by a finite heat flux temperature gradient at the left hand boundary, where the temperature has its maximum value. In the present rotation

$$\theta(x;\ell) = a(1 - x) + \ell n\ \ell, \qquad \text{(C.5.20)}$$

where a is a positive constant. From (C.5.11) it follows that

$$t_e = \frac{1}{\ell} \exp(-a(1-x)), \qquad \text{(C.5.21)}$$

with a minimum ignition time

$$t_{eo} = \frac{1}{\ell}\, e^{-a} \qquad \text{(C.5.22)}$$

on $x = 0$.

Type I is characterized by zero heat flux at the left hand boundary where again the temperature has its maximum value. For this case JKS take

$$\theta(x;\ell) = a(1-x^2) + \ell n\ \ell, \tag{C.5.23}$$

for which

$$t_e(x) = \frac{1}{\ell} \exp\left[-a(1-x^2)\right] \tag{C.5.24}$$

and again t_{eo} is the minimum ignition time on $x = 0$.

Both cases correspond to initiating hot spots at $x = \tau = 0$. As in §3, the ignition time on $x = 0$ can be found from the expansion

$$t_i = t_{eo} + \delta t_{e1} + \ \ldots\ . \tag{C.5.25}$$

Determination of t_{e1} requires an analysis of the behavior of (C.5.19) near the hot spot. Based on the results of Friedman & Herrera, it is required that the local singular behavior is, at most, logarithmic. After some analysis (Crighton & Blythe, 1993) it can be established that

$$t_{e_1} = -\int_o^{t_{eo}} t_{1o}\,(0,s)\ ds. \tag{C.5.27}$$

If the constants ℓ and a are such that $t_{eo} < 1$, then $(0 < t < 1)$

$$p_{1o}(0,t) = \frac{1}{2} f(t) = \int_o^t \frac{ds}{t_e(s) + s - t}\ . \tag{C.5.28}$$

For type B profiles JKS give, for $a = 0.5$ and $\ell = 0.8$,

$$t_i = 0.447, \tag{C.5.29}$$

while the present analytical approach yields

$$t_i = 0.461\ + O(\delta^2). \tag{C.5.30}$$

Both of these results are based on $\gamma = 7/5$ so that $\delta = 2/7$. In view of the size of δ, the agreement between (C.5.29) and (C.5.30) is remarkably good. Comparison between the predicted temperature distribution and JKS shows even better agreement. Details are provided in Crighton & Blythe (1993). Calculations for type I profiles are currently in progress.

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